

Néel state of antiferromagnet as a result of a local measurement in the distributed quantum system

M. I. Katsnelson*, V. V. Dobrovitski, and B. N. Harmon

Ames Laboratory, Iowa State University, Department of Physics and Astronomy, Ames, Iowa, 50011
(today)

Single-site measurement in a distributed macroscopic antiferromagnet is considered; we show that it can create antiferromagnetic sublattices at macroscopic scale. We demonstrate that the result of measurement depends on the symmetry of the ground state: for the easy-axis case the Néel state is formed, while for the easy-plane case unusual “fan” sublattices appear with unbroken rotational symmetry, and a decoherence wave is generated. For the latter case, a macroscopically large number of measurements is needed to pin down the orientation of the sublattices, in spite of the high degeneracy of the ground state. We note that the type of the final state and the appearance of the decoherence wave are governed by the degree of entanglement of spins in the system.

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The ordered antiferromagnetic (AFM) state has been extensively discussed since the experimental discovery of antiferromagnetism [1,2]. The conventional picture, associated with L. Néel, represents a macroscopic antiferromagnet as consisting of two sublattices, each possessing a macroscopically large total spin \mathbf{S}_A . This picture agrees with the experiments on macroscopic antiferromagnets [2], but serious conceptual problems arise. The ground state of a Heisenberg magnet with AFM exchange interactions should be a nondegenerate singlet with zero total magnetization of each sublattice. Moreover, the AFM ground state should be time-reversal invariant, while the Néel state is obviously not. For a long time, it was commonly believed that the difficulty can be resolved by recognizing that due to very high (quasi)degeneracy of the AFM ground state (the separation between the lowest levels is of order $1/N$, where N is the total number of spins in the sample), “extremely weak forces can pin down the orientation” (quote from Ref. [3]) of the sublattices thus breaking the rotational and time-reversal symmetries and leading to the Néel state. Latter advances in quantum measurement theory [4] demonstrated that it is not the interaction strength itself that matters, but its ability to build up quantum correlations (entanglement) between the system and its environment, so that the system decoheres and the initial symmetry breaks. In many realistic situations, the process of decoherence is extremely fast, and can be considered as a quantum measurement in the von Neumann’s sense [5], i.e. as an instantaneous projection of the system’s initial state onto the final state with broken symmetry.

However, in the present paper, we show that building the argument upon quasidegeneracy is intrinsically misleading. We present two situations, realistically modeling easy-plane and easy-axis antiferromagnets, which have the same quasidegeneracy (with the lowest levels separation $1/N$), and we show that the impact of environmental measurement on each of the systems is drastically different: although time-reversal symmetry breaks in both cases, this is not so for the rotational symmetry, i.e. sublattices can emerge without formation of the Néel state, leaving the orientation of sublattices magnetization indeterminate. We show that the different scenarios take place because of different degrees of entanglement between the individual spins in an antiferromagnet.

Appearance of the AFM sublattices due to environmental “measurement” has been studied [6] for the case of very small antiferromagnetic particles using the method of collective coordinate, by mapping of the low-energy part of the antiferromagnet’s spectrum onto a two-state system [7]. Such a mapping is valid when all the excited states are well-separated from the doublet of lowest levels, and the non-collective dynamics can be neglected, i.e. in the case of easy-axis antiferromagnet with noticeable anisotropy. But in macroscopic samples the well-separated ground doublet can be absent (e.g., the long-wavelength magnons in the easy-plane antiferromagnet are gapless, and corresponding excitations can be very close to the ground state), and the mapping onto a two-state system is not legitimate. Also, measurement in a distributed quantum system often generates a decoherence wave [9] which can not be described by the collective coordinate method. Furthermore, in reality, the interactions with dissipative degrees of freedom, such as nuclear spins, are short-ranged, so that corresponding measurements are essentially *local*. Locality of the measurement, which discriminates the given site (belonging to the sublattice A) from its neighbors (belonging to the sublattice B), is crucial; the global measurement which does not distinguish sites from different sublattices can not resolve the Néel state and can not cause the formation of sublattices [8].

Therefore, to describe the appearance of sublattices, we have to consider *local* measurement in a *distributed* quantum spin system. To our knowledge, this problem has never been applied before to the study of antiferromagnets. In this paper, we show that even the microscopic single-site measurement can create sublattices

in the macroscopically large antiferromagnet which was initially in the time-reversal-symmetric state. We study this process in detail and show that it can be very different from what is suggested by the collective coordinate method or similar models.

Let us consider the Heisenberg antiferromagnet containing N sites with the spin S at each site; the isotropic exchange part of its Hamiltonian is

$$\mathcal{H}_0 = \sum_{\mathbf{q}} J_{\mathbf{q}} (S_{\mathbf{q}}^+ S_{-\mathbf{q}}^- + S_{\mathbf{q}}^z S_{-\mathbf{q}}^z), \quad (1)$$

where $S_{\mathbf{q}}^+ = (1/\sqrt{N}) \sum_j s_j^+ \exp(i\mathbf{q}\mathbf{r}_j)$, and, similarly, $S_{\mathbf{q}}^-$ and $S_{\mathbf{q}}^z$ are the Fourier transforms of the single-site spin operators: s_j^+ and s_j^- are the ladder spin operators for the site j , and s_j^z is the operator of the z -projection of the spin at the site j . Analogously, $J_{\mathbf{q}}$ is the Fourier transform of the exchange integral, where $\sum_{\mathbf{q}} J_{\mathbf{q}} = 0$. If the exchange integrals are such that $\max_{\mathbf{q}} J_{\mathbf{q}} = J_{\mathbf{Q}}$ and $2\mathbf{Q}$ coincides with the vector of the reciprocal lattice, then the AFM ordering appears along the vector \mathbf{Q} ; we assume infinite correlation length since the finite-temperature effects are beyond the scope of this paper.

As will be shown below, it is important to take into account the symmetry of the ground state imposed by the anisotropic interactions, so we assume a very small anisotropy term \mathcal{H}' , e.g., of the form $\mathcal{H}' = D \sum_j (s_j^z)^2$, also present in the system's Hamiltonian. It can be seen that for very small D the analysis given below does not depend on the specific form of the anisotropy, nor on its magnitude: symmetry of the ground state is predominant, so we assume $D \rightarrow \pm 0$ below.

First, let us consider the case of easy-plane anisotropy, $D \rightarrow +0$. Exact eigenstates of the system are not known, except for some very special situations. To describe AFM states in the general case, the following family of time-reversal-symmetric (TRS) states has been proposed [8]:

$$|\Psi_M\rangle = \left[\frac{N^M (2NS - M)!}{M! (2NS)!} \right]^{1/2} (S_{\mathbf{Q}}^-)^M |0\rangle \quad (2)$$

where $M = 0, \dots, 2NS$ is an integer, and $|0\rangle$ is the ferromagnetic state (all spins up). The state $|\Psi_M\rangle$ is an eigenstate of the z -projection of the operator of the total system's spin with the eigenvalue $S_z = NS - M$, so the AFM ground state corresponds to $M = NS$. The state (2) can be considered as the time-reversal-symmetric counterpart of the Néel state: both of them have the same energy, the same correlation functions, etc., and they can not be distinguished by conventional experimental means (such as neutron scattering or NMR). Moreover, the energy of the TRS-state is very close to the energy of the exact AFM ground state: they differ by terms of order of $1/(zS)$ where z is the coordination number [1] which is often large (e.g., $z = 8$ for *bcc* lattice). For simplicity, below we consider only the case $S = 1/2$, so that our treatment can be considered as formally rigorous in the limit

$z \rightarrow \infty$, i.e. for infinite-dimensional space. Note that the difference in energy between the states $|\Psi_M\rangle$ with M close to NS is of order $1/N$, i.e. the ground state is highly (quasi)degenerate.

Below, to characterize the states of the antiferromagnet, it is convenient to use the correlation functions $K^{\alpha\beta}(\mathbf{q}) = \text{Tr}[\rho S_{\mathbf{q}}^{\alpha} S_{-\mathbf{q}}^{\beta}]$, where ρ is the density matrix. For the state (2) we have

$$\begin{aligned} K_i^{+-}(\mathbf{q}) &= \langle S_{\mathbf{q}}^+ S_{-\mathbf{q}}^- \rangle = NS^2 \delta_{\mathbf{q}\mathbf{Q}} + S/2, \\ K_i^{zz}(\mathbf{q}) &= \langle S_{\mathbf{q}}^z S_{-\mathbf{q}}^z \rangle = S/2, \end{aligned} \quad (3)$$

where the subscript i stands for the initial state, and this state can be imagined as a state with all the spins aligned antiferromagnetically along some AFM axis (note the delta-functional singularity in K^{+-}), but the axis itself is uniformly smeared in the x - y plane, see Fig. 1a. Obviously, in this state the sublattices are absent.

Now, suppose that we perform a local measurement of the spin x -projection at the site 0. In reality, no conscious effort is needed for that, since the electronic spin at every site interacts with its environment (e.g., a nuclear spin at this site), so the initial state of the electronic spin decoheres [4], i.e., the environment acts as a measuring apparatus. Decoherence of the single spin by its environment can be described following the Ref. [6]; in many realistic cases this process is very fast, so we describe it using von Neumann's theory, as a projection of the initial state onto the eigenstates of the operator s_0^x . Therefore, the system occurs in a mixed quantum state which is described by the density matrix

$$\begin{aligned} \rho_f &= (|\Phi^+\rangle\langle\Phi^+| + |\Phi^-\rangle\langle\Phi^-|), \\ |\Phi^{\pm}\rangle &= W^{\pm} |\Psi_M\rangle = \left(\frac{1}{2} \pm s_0^x \right) |\Psi_M\rangle, \end{aligned} \quad (4)$$

where, for $S = 1/2$, W^+ and W^- are the projectors onto the eigenstates of s_0^x with the eigenvalues $+1/2$ and $-1/2$ respectively. The function $|\Phi^+\rangle$ ($|\Phi^-\rangle$) describes the state of the sample after the measurement, provided that the measurement gave the result $+1/2$ ($-1/2$). Note that the norm of both $|\Phi^+\rangle$ and $|\Phi^-\rangle$ is $1/2$, i.e. each state appears with the probability $1/2$. The calculations give the explicit form:

$$\begin{aligned} |\Phi^{\pm}\rangle &= |\Phi_{\text{coh}}^{\pm}\rangle + |\Phi_{\text{inc}}^{\pm}\rangle, \\ |\Phi_{\text{coh}}^{\pm}\rangle &= \frac{1}{2} |\Psi_M\rangle \pm \frac{1}{2} (\alpha_M |\Psi_{M-1}\rangle + \alpha_{M+1} |\Psi_{M+1}\rangle), \\ |\Phi_{\text{inc}}^{\pm}\rangle &= \pm \frac{1}{2\sqrt{N}} \sum_{\mathbf{q} \neq \mathbf{Q}} S_{\mathbf{q}}^- (|\Psi_M\rangle - \gamma_M |\Psi_{M-2}\rangle), \end{aligned} \quad (5)$$

where $|\Phi_{\text{coh}}^{\pm}\rangle$ represents contributions from the states with $\mathbf{q} = \mathbf{Q}$, while $|\Phi_{\text{inc}}^{\pm}\rangle$ corresponds to the excitations with $\mathbf{q} \neq \mathbf{Q}$, and $\alpha_M = \sqrt{M(N-M+1)/N^2}$, $\gamma_M = \sqrt{M(M-1)/[(N-M+1)(N-M+2)]}$.

The initial AFM ground state is invariant with respect to rotations in the x - y plane, and so is the final state produced by the measurement:

$$\begin{aligned} K_f^{+-}(\mathbf{Q}) &= K_f^{xx}(\mathbf{Q}) + K_f^{yy}(\mathbf{Q}) = N/4, \\ K_f^{--}(\mathbf{Q}) &= K_f^{xx}(\mathbf{Q}) - K_f^{yy}(\mathbf{Q}) = 1/16, \end{aligned} \quad (6)$$

for $N \gg 1$, where we took into account that $M = NS$ for the AFM ground state. Only the direction of the measured spin at the site $j = 0$ is fixed, while for the rest of the sample the AFM axis in the x - y plane is not fixed. This is quite different from what is predicted by the collective coordinate approach [6] or other models such as the classical σ -model.

However, in spite of the indeterminate AFM axis, sublattices are *created* in the sample. Indeed, for every site j ($j \neq 0$):

$$\langle s_j^x \rangle_{\pm} = \frac{\langle \Phi^{\pm} | s_j^x | \Phi^{\pm} \rangle}{\langle \Phi^{\pm} | \Phi^{\pm} \rangle} = \pm \frac{1}{4} \exp(-i\mathbf{Q}\mathbf{r}_j) \quad (7)$$

i.e., for each result of the measurement, the x -component of the spin at every site is nonzero, although twice smaller than for the Néel state, and the spins are ordered antiferromagnetically. This state can be interpreted in quasi-classical terms as an AFM “fan” structure, where due to the measurement the spins at the sites $j \neq 0$ are localized essentially within the semicircles, but their direction inside the semicircles is not fixed (see Fig. 1b). This picture can be confirmed by calculation of other quantities (the amplitude $\langle S_{\mathbf{Q}}^x \rangle$ of the mode $\mathbf{q} = \mathbf{Q}$, single-spin density matrix, etc.).

Now, let us consider the case of the easy-axis anisotropy, assuming that the easy axis is directed along the x -axis. The TRS ansatz for the corresponding AFM ground state is [8]

$$|\Psi\rangle = \sum_{L=0}^{2NS} u_L |\Psi_{2L}\rangle, \quad \sum_{L=0}^{2NS} u_L^2 = 1, \quad (8)$$

where $u_L = \exp[\phi(L)/2]$, and $\phi(L)$ is some real function, whose explicit form is immaterial in the limit $N \rightarrow \infty$ provided that it has a well-pronounced maximum in the neighborhood of $L_0 = NS$. It has been shown [8] that this state corresponds to the AFM state without sublattices, but with the AFM ordering axis directed along the x -axis. As above, we consider the state of the system after the measurement made on the x -component of the spin at the site $j = 0$. The resulting density matrix is $\rho_f = |\Phi^+\rangle\langle\Phi^+| + |\Phi^-\rangle\langle\Phi^-|$, and in the thermodynamic limit

$$|\Phi^{\pm}\rangle = \frac{1}{2} \sum_L u_L [|\Psi_{2L}\rangle \pm \alpha_{2L+1} |\Psi_{2L+1}\rangle \pm \alpha_{2L} |\Psi_{2L-1}\rangle] \quad (9)$$

while the excitations with $\mathbf{q} \neq \mathbf{Q}$ are negligible. It can be checked that the resulting state is, in fact, the Néel state: e.g., the x -component of the spin at the site j is $\langle s_j^x \rangle_{\pm} = \pm(1/2) \exp(-i\mathbf{Q}\mathbf{r}_j)$, exactly as in the Néel state (see Fig. 1d).

Therefore, for the antiferromagnet which is initially in the TRS-state, even the single site measurement can create sublattices over the whole sample. However, these sublattices have the usual Néel form only for the easy-axis antiferromagnet. For the easy-plane antiferromagnet, the “fan” sublattices appear, where the AFM axis is indeterminate in the x - y plane, and each spin is directed up or down only in average, being localized essentially in the semicircle. Our conclusions do not depend on the specific form of the anisotropic term in the Hamiltonian, and are based only on the use of the TRS-states for description of the AFM ground state. This description is expected to be valid for small anisotropy with accuracy of order $1/(zS)$. As a rule, this approximation works well [10].

To produce the Néel state in the easy-plane case, a macroscopically large number of further measurements are necessary. Indeed, every measurement admixes to the initial state $|\Psi_M\rangle$ the states $|\Psi_{M\pm 1}\rangle$, so that to encompass all values of M and fix the direction of the AFM axis, we need of order of $N/2$ measurements. Informally, it can be understood by taking into account the uncertainty relation for the z -projection of the total spin S_z and the angle ϕ of AFM axis in the x - y plane: $\Delta S_z \Delta \phi \sim 1$. The value of ϕ becomes certain when ΔS_z is maximal. This situation is analogous to the case of Bose-Einstein condensate, where the well-defined phase is built up by increasing uncertainty in the number of particles [11].

Nevertheless, appearance of the sublattices is not the whole story. It has been shown [9] that the local measurement in a distributed quantum system creates a decoherence wave propagating in the system. In the antiferromagnet, the decoherence wave can be created only by the contributions with $\mathbf{q} \neq \mathbf{Q}$: the excitations with $\mathbf{q} = \mathbf{Q}$ are static (have zero frequency). For example, in the easy-plane case $\langle s_j^x \rangle(t) = \pm \text{Re}\langle s_j^+(t) s_0^- \rangle$, i.e. the local spin measurement induces the decoherence wave, and its dynamics is governed by the Green’s function $G(\mathbf{r}_{jk}, t) = \langle s_j^+(t) s_k^- \rangle - \langle s_j^+ s_k^- \rangle$. For the easy-plane TRS-state $G(\mathbf{r}, t)$ can not be calculated exactly, but estimates based on the magnon picture give $G(\mathbf{r}, t) = (4N)^{-1} \sum_{\mathbf{q}} \exp[i\mathbf{q}\mathbf{r} - i\omega_{\mathbf{q}} t]$, where $\omega_{\mathbf{q}} = \sqrt{(J_{\mathbf{Q}} - J_{\mathbf{q}})(J_{\mathbf{Q}} - J_{\mathbf{q}-\mathbf{Q}})}$ is the frequency of antiferromagnons. It is worth noting that the decoherence wave appears only in the easy-plane case, where the localization of the AFM axis is incomplete. In the easy-axis case the AFM axis is localized completely but the incoherent contribution in the wave function is negligible in the limit $N \rightarrow \infty$, so the decoherence wave is absent. This corroborates the conjecture [9] that the decoherence

wave is the result of incomplete entanglement between the entities comprising the system. Indeed, in the easy-axis case the entanglement is complete, and measurement of the direction of one spin determines the direction of every other spin in the sample. In the easy-plane case, the entanglement is not so constraining, so that the excitations with $\mathbf{q} \neq \mathbf{Q}$ emerge, making the AFM axis indeterminate and giving rise to the decoherence wave.

Results of the present paper can have also experimental importance. At present, there is a growing interest in antiferromagnetic systems of significant size which, nonetheless, demonstrate quantum coherence. Mention can be made of the single-molecule antiferromagnets [12] Fe_{10} , Fe_6 , etc. Another relevant class of experimentally interesting systems is the artificial spin rings made of paramagnetic atoms to form a “quantum corral” [13]. Noticeable AFM interactions can exist between the spins in this system, while major sources of decoherence, nuclear spins and conduction electrons [6], can be avoided, e.g., by using iron atoms and silicon substrate at low temperatures. The spin state of the atoms in the ring can be probed by scanning tunneling microscopy which can provide [14] the spatial resolution of ca. 10 Å and sensitivity of order of few Bohr’s magnetons, or by magnetic resonance force microscopy [15]. But development and analysis of realistic experimental schemes constitutes a distinct problem, requiring separate detailed study, and we do not discuss it here.

Summarizing, we have shown that the *local* measurement in a distributed macroscopic antiferromagnet can create sublattices in the whole sample. Therefore, considering the sublattices as a result of decoherence, it is not necessary to presume a measurement embracing the whole macroscopic sample at once. We show that the result of measurement depends on the symmetry of the ground state. For the easy-axis case the collective coordinate approach gives essentially the complete picture, with both time-reversal and rotational symmetries broken. For the easy-plane case, unusual “fan” sublattices appear, i.e. only time-reversal symmetry breaking takes place while rotational symmetry is preserved (in spite of high degeneracy of the ground state); moreover, in this case a decoherence wave is generated by measurement. We conclude that both the certainty of the final state and the appearance of the decoherence wave are governed by the degree of entanglement of spins in the system.

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* Permanent address: Institute of Metal Physics, Ekaterinburg 620219 Russia.

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FIG. 1. Sketch of the spin arrangement. Easy plane case: (a) before measurement spins are antiferromagnetically ordered, but sublattices are absent and the total AFM axis is not fixed; (b) after measurement the “fan” sublattices emerge but AFM axis is not fixed. Easy axis case: (c) before measurement spins are directed along *x*-axis but sublattices are absent; (d) after measurement the Néel state appears.

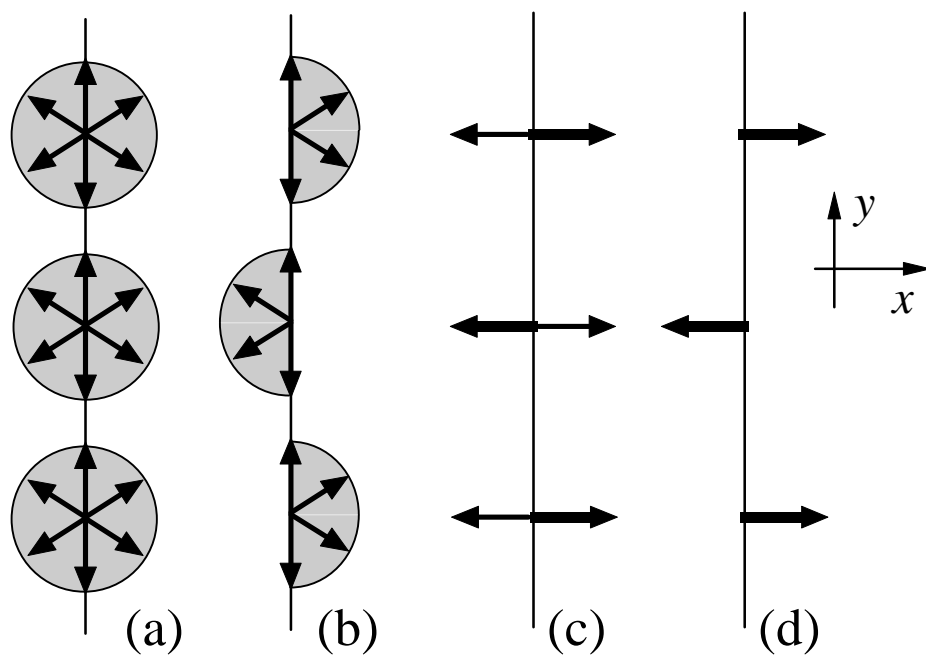


Fig. 1

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“Neel state of antiferromagnet ...”